



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:19 AM UTC

PDB ID : 9VJJ / pdb_00009vjj
Title : Crystal Structure of human Latent TGF-beta1 in complex with SOF10
Authors : Kawauchi, H.; Kanamori, M.; Sato, I.; Fukami, T.A.; Irie, M.; Torizawa, T.; Shimada, H.
Deposited on : 2025-06-20
Resolution : 2.48 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

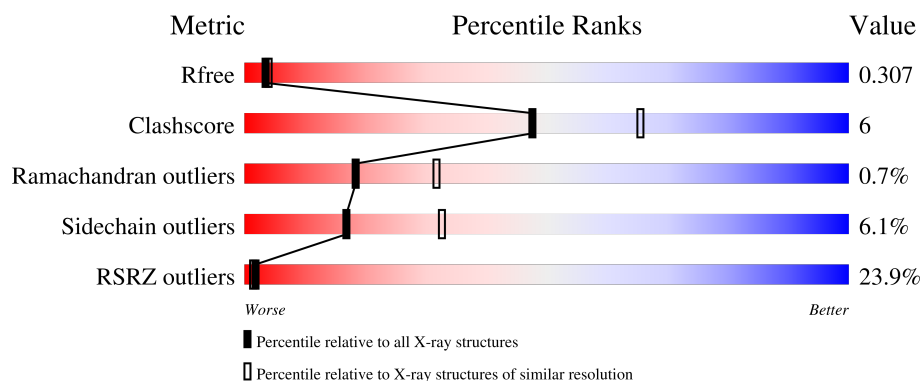
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	369	21% 64% 16% • 18%
1	B	369	21% 69% 16% • 14%
2	H	227	7% 46% 8% 46%
2	I	227	21% 44% 8% • 47%
3	L	215	4% 42% 7% 50%

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Mol	Chain	Length	Quality of chain
3	M	215	13% 39% 10% 50%
4	C	2	100%
4	D	2	100%
4	E	2	50% 50%
4	X	2	50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8418 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transforming growth factor beta-1 proprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2380	1514	414	436	16			
1	B	317	Total	C	N	O	S	0	0	0
			2475	1577	425	456	17			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ASP	-	expression tag	UNP P01137
A	23	TYR	-	expression tag	UNP P01137
A	24	LYS	-	expression tag	UNP P01137
A	25	ASP	-	expression tag	UNP P01137
A	26	ASP	-	expression tag	UNP P01137
A	27	ASP	-	expression tag	UNP P01137
A	28	ASP	-	expression tag	UNP P01137
A	29	LYS	-	expression tag	UNP P01137
A	33	SER	CYS	engineered mutation	UNP P01137
B	22	ASP	-	expression tag	UNP P01137
B	23	TYR	-	expression tag	UNP P01137
B	24	LYS	-	expression tag	UNP P01137
B	25	ASP	-	expression tag	UNP P01137
B	26	ASP	-	expression tag	UNP P01137
B	27	ASP	-	expression tag	UNP P01137
B	28	ASP	-	expression tag	UNP P01137
B	29	LYS	-	expression tag	UNP P01137
B	33	SER	CYS	engineered mutation	UNP P01137

- Molecule 2 is a protein called SOF10 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	122	Total	C	N	O	S	0	0	0
			940	600	157	178	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	121	Total	C	N	O	S	0	0	0
			926	591	155	175	5			

- Molecule 3 is a protein called SOF10 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	107	Total	C	N	O	S	0	0	0
			795	497	126	169	3			
3	M	107	Total	C	N	O	S	0	0	0
			786	493	124	166	3			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	X	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

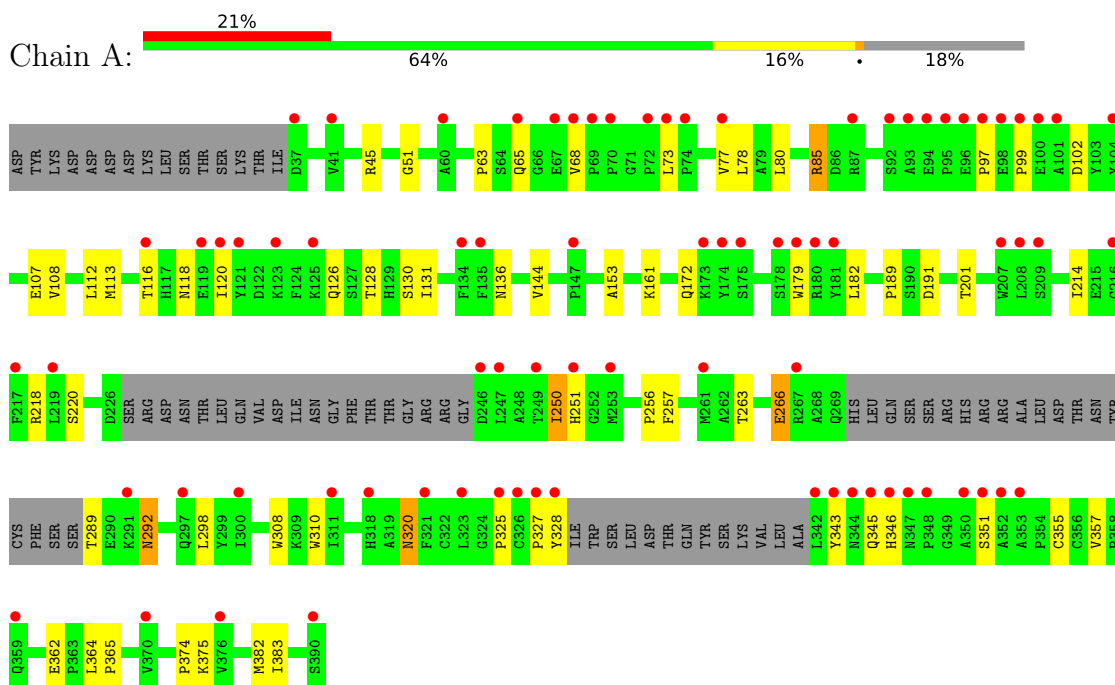
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total O 2 2	0	0
5	L	1	Total O 1 1	0	0
5	M	1	Total O 1 1	0	0

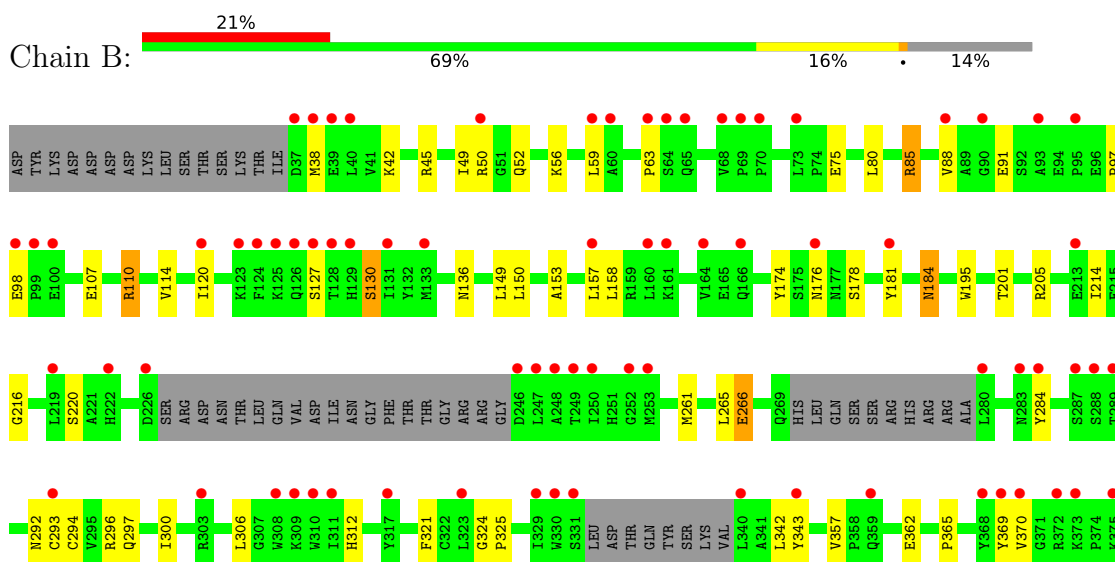
3 Residue-property plots

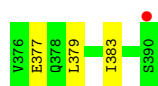
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Transforming growth factor beta-1 proprotein



- Molecule 1: Transforming growth factor beta-1 proprotein

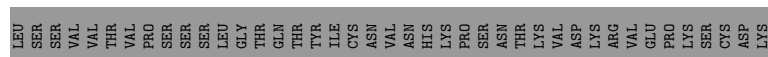
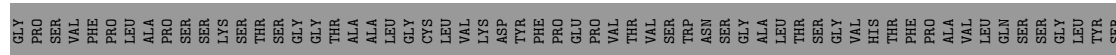
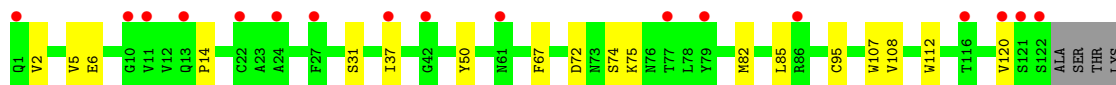




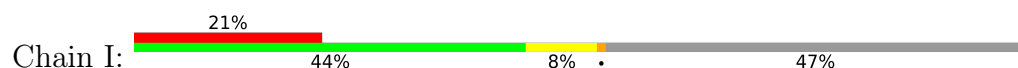
- Molecule 2: SOF10 Fab heavy chain



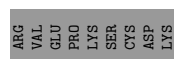
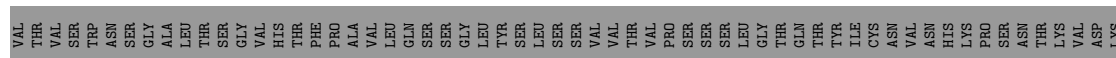
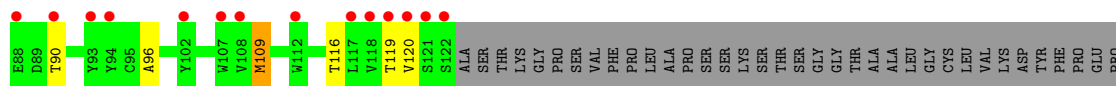
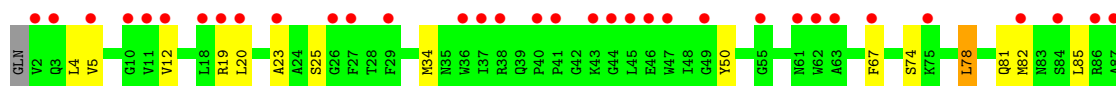
Chain H:



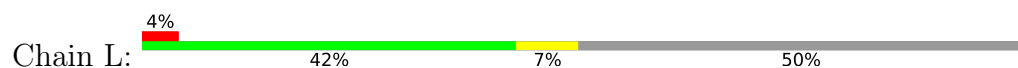
- Molecule 2: SOF10 Fab heavy chain



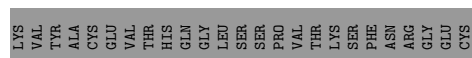
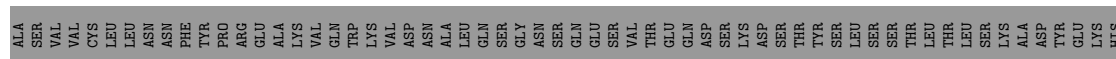
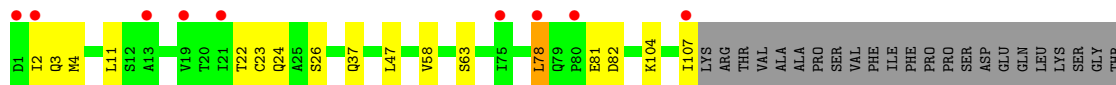
Chain I:



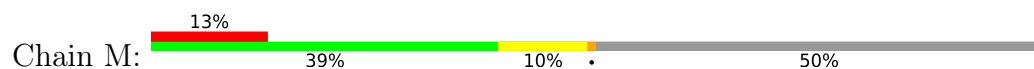
- Molecule 3: SOF10 Fab light chain



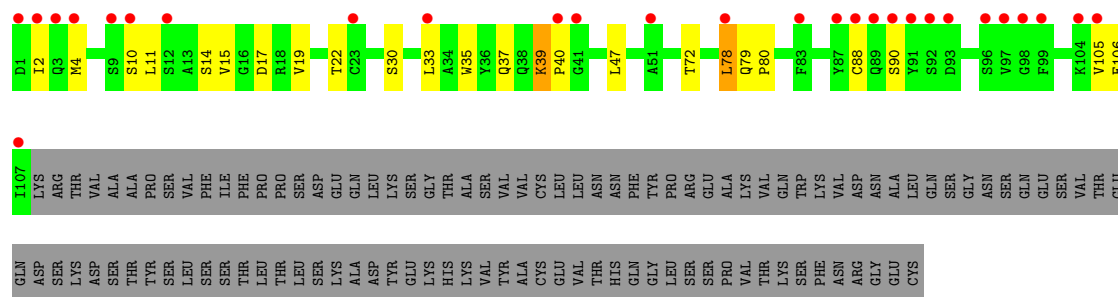
Chain L:



- Molecule 3: SOF10 Fab light chain



Chain M:



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 50% 50%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.88Å 91.71Å 126.12Å 90.00° 108.58° 90.00°	Depositor
Resolution (Å)	36.12 – 2.48 36.12 – 2.48	Depositor EDS
% Data completeness (in resolution range)	62.9 (36.12-2.48) 62.9 (36.12-2.48)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.281 , 0.310 0.279 , 0.307	Depositor DCC
R_{free} test set	2765 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	77.7	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8418	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.73	0/2440	1.06	4/3319 (0.1%)
1	B	0.76	0/2539	1.10	8/3459 (0.2%)
2	H	0.73	0/966	0.97	1/1318 (0.1%)
2	I	0.65	0/952	0.96	0/1301
3	L	0.71	0/812	0.99	0/1105
3	M	0.70	1/803 (0.1%)	0.95	0/1094
All	All	0.73	1/8512 (0.0%)	1.04	13/11596 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	39	LYS	CA-C	5.03	1.59	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASN	CA-CB-CG	6.27	118.87	112.60
1	B	130	SER	N-CA-C	5.67	117.90	108.99
1	B	284	TYR	CA-C-N	5.59	128.04	120.44
1	B	284	TYR	C-N-CA	5.59	128.04	120.44
1	B	216	GLY	N-CA-C	5.58	120.58	111.27
1	B	91	GLU	N-CA-C	5.55	117.33	111.28
1	B	136	ASN	CA-C-N	5.44	128.11	120.28
1	B	136	ASN	C-N-CA	5.44	128.11	120.28
1	A	68	VAL	N-CA-C	5.33	113.14	107.76
1	B	184	ASN	CA-CB-CG	5.30	117.90	112.60
2	H	108	VAL	N-CA-C	-5.12	99.79	107.37
1	A	266	GLU	CA-C-N	5.01	127.50	120.28
1	A	266	GLU	C-N-CA	5.01	127.50	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2380	0	2299	36	0
1	B	2475	0	2347	32	0
2	H	940	0	880	9	0
2	I	926	0	858	9	0
3	L	795	0	755	5	0
3	M	786	0	740	10	0
4	C	28	0	25	0	0
4	D	28	0	25	1	0
4	E	28	0	25	0	0
4	X	28	0	25	0	0
5	B	2	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
All	All	8418	0	7979	91	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (91) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ASN:HA	1:A:325:PRO:HD2	1.36	1.05
1:B:292:ASN:HA	1:B:325:PRO:HD2	1.47	0.96
1:A:116:THR:HG21	1:A:251:HIS:CE1	2.06	0.90
1:B:158:LEU:HD13	1:B:195:TRP:CE2	2.11	0.86
1:A:97:PRO:HD3	2:I:74:SER:HA	1.60	0.84
1:B:130:SER:HB3	1:B:220:SER:HA	1.59	0.82
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.62	0.79
1:B:85:ARG:HB3	1:B:365:PRO:HG2	1.66	0.76
3:M:39:LYS:HB3	3:M:40:PRO:HD2	1.68	0.76
1:B:97:PRO:HD3	2:H:74:SER:HA	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:THR:HG21	1:A:251:HIS:ND1	2.06	0.70
1:A:375:LYS:HE3	1:B:107:GLU:HG3	1.82	0.62
1:B:312:HIS:NE2	1:B:369:TYR:HD2	1.98	0.62
2:I:90:THR:HG23	2:I:119:THR:HA	1.80	0.62
1:B:181:TYR:OH	1:B:184:ASN:HB3	1.99	0.62
3:M:37:GLN:HB2	3:M:47:LEU:HD11	1.82	0.61
3:L:4:MET:HE3	3:L:23:CYS:SG	2.41	0.61
1:A:218:ARG:NH1	1:A:220:SER:OG	2.34	0.60
1:A:120:ILE:HD13	1:A:214:ILE:HD13	1.84	0.60
1:A:107:GLU:HA	1:B:377:GLU:HG2	1.85	0.59
3:M:79:GLN:HB3	3:M:80:PRO:HD2	1.85	0.59
3:M:39:LYS:HB3	3:M:40:PRO:CD	2.33	0.58
1:A:112:LEU:HD13	1:A:257:PHE:HB3	1.86	0.58
1:B:150:LEU:O	1:B:205:ARG:NH2	2.39	0.56
2:I:20:LEU:HD13	2:I:82:MET:HE1	1.89	0.55
1:A:172:GLN:HB2	1:A:182:LEU:HD11	1.89	0.55
1:B:56:LYS:HD3	1:B:379:LEU:HD12	1.88	0.55
2:H:82:MET:HE2	2:H:85:LEU:HD21	1.89	0.54
2:I:96:ALA:HB1	2:I:109:MET:HB3	1.89	0.54
1:A:345:GLN:NE2	1:A:346:HIS:HE1	2.06	0.53
1:A:131:ILE:HD12	1:A:250:ILE:HD11	1.90	0.53
2:I:5:VAL:HG23	2:I:23:ALA:HB3	1.89	0.53
1:A:99:PRO:HG2	1:A:102:ASP:HB2	1.92	0.52
1:A:126:GLN:O	1:A:130:SER:O	2.28	0.52
3:L:3:GLN:HB2	3:L:26:SER:HB3	1.92	0.52
1:A:298:LEU:H	1:A:320:ASN:HD22	1.57	0.51
1:A:345:GLN:NE2	1:A:346:HIS:CE1	2.78	0.51
1:A:130:SER:HB3	1:A:220:SER:HA	1.93	0.51
1:B:59:LEU:HD13	1:B:63:PRO:HD3	1.93	0.51
1:B:50:ARG:HB2	1:B:306:LEU:HD22	1.93	0.51
2:I:12:VAL:HG21	2:I:85:LEU:HD13	1.92	0.50
1:B:38:MET:HE3	1:B:42:LYS:HE3	1.93	0.50
1:B:312:HIS:NE2	1:B:369:TYR:CD2	2.79	0.50
1:A:116:THR:HG21	1:A:251:HIS:HE1	1.69	0.49
1:A:80:LEU:HD13	1:B:110:ARG:HB3	1.93	0.49
1:B:149:LEU:HD11	1:B:265:LEU:HD13	1.94	0.49
2:I:19:ARG:HG3	2:I:81:GLN:HG2	1.94	0.49
1:A:113:MET:HE2	1:A:256:PRO:HD2	1.95	0.49
1:A:364:LEU:HB3	1:A:382:MET:HG3	1.95	0.49
1:B:174:TYR:O	1:B:178:SER:HB2	2.13	0.48
2:H:14:PRO:HG3	2:H:120:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:19:VAL:HG21	3:M:78:LEU:HD22	1.95	0.47
1:B:52:GLN:HG2	1:B:56:LYS:HD2	1.97	0.47
2:I:34:MET:HB3	2:I:78:LEU:HD22	1.97	0.46
1:A:362:GLU:HB2	1:A:383:ILE:HB	1.97	0.46
3:M:11:LEU:HB3	3:M:105:VAL:HG12	1.98	0.46
1:A:108:VAL:O	1:B:80:LEU:HD21	2.16	0.45
1:A:85:ARG:HB3	1:A:365:PRO:HG2	1.99	0.45
1:A:77:VAL:HG21	1:A:374:PRO:HG2	1.98	0.45
1:B:158:LEU:HD13	1:B:195:TRP:CD2	2.49	0.45
1:A:189:PRO:HG2	2:H:107:TRP:CH2	2.51	0.44
1:A:266:GLU:H	1:A:266:GLU:CD	2.25	0.44
3:L:78:LEU:HD12	3:L:82:ASP:HB2	1.99	0.44
1:B:296:ARG:HB2	1:B:321:PHE:CZ	2.52	0.44
1:A:327:PRO:HD2	1:A:346:HIS:CE1	2.52	0.44
1:B:362:GLU:HB2	1:B:383:ILE:HB	1.99	0.44
1:B:293:CYS:HA	1:B:324:GLY:HA3	1.99	0.44
2:I:67:PHE:CE2	2:I:82:MET:HG2	2.53	0.43
3:M:4:MET:HE3	3:M:90:SER:HB3	1.99	0.43
1:B:266:GLU:H	1:B:266:GLU:CD	2.26	0.43
1:A:308:TRP:CG	1:A:310:TRP:HE1	2.37	0.43
2:H:67:PHE:CE2	2:H:82:MET:HG2	2.54	0.43
3:M:22:THR:HG22	3:M:72:THR:HG22	2.00	0.42
1:A:153:ALA:HB3	1:A:201:THR:HA	2.01	0.42
1:A:161:LYS:HG3	1:A:191:ASP:HA	2.01	0.42
1:B:49:ILE:HG21	1:B:300:ILE:HD13	2.02	0.42
1:A:51:GLY:HA3	1:B:343:TYR:CZ	2.55	0.42
1:A:116:THR:CG2	1:A:251:HIS:ND1	2.78	0.42
1:A:357:VAL:HG21	1:B:357:VAL:HG21	2.02	0.42
1:B:97:PRO:HD3	2:H:74:SER:CA	2.44	0.42
2:H:6:GLU:OE2	2:H:95:CYS:SG	2.78	0.42
2:H:72:ASP:CG	2:H:75:LYS:HG3	2.45	0.41
1:B:214:ILE:HD11	4:D:1:NAG:H82	2.01	0.41
3:M:35:TRP:CZ3	3:M:88:CYS:HB3	2.56	0.41
1:B:153:ALA:HB3	1:B:201:THR:HA	2.02	0.41
1:A:45:ARG:HG2	1:A:298:LEU:CD2	2.51	0.41
1:A:179:TRP:CG	1:A:218:ARG:HH21	2.38	0.41
2:H:37:ILE:HD13	2:H:112:TRP:CZ3	2.55	0.41
3:M:15:VAL:HA	3:M:78:LEU:O	2.21	0.41
3:L:47:LEU:HA	3:L:58:VAL:HG21	2.03	0.41
1:B:370:VAL:HG23	1:B:370:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/369 (80%)	273 (92%)	18 (6%)	4 (1%)	9	15
1	B	309/369 (84%)	285 (92%)	23 (7%)	1 (0%)	36	53
2	H	120/227 (53%)	116 (97%)	4 (3%)	0	100	100
2	I	119/227 (52%)	112 (94%)	7 (6%)	0	100	100
3	L	105/215 (49%)	100 (95%)	4 (4%)	1 (1%)	12	22
3	M	105/215 (49%)	91 (87%)	13 (12%)	1 (1%)	12	22
All	All	1053/1622 (65%)	977 (93%)	69 (7%)	7 (1%)	18	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	78	LEU
1	A	128	THR
1	A	320	ASN
1	B	127	SER
1	A	63	PRO
1	A	292	ASN
3	M	78	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	256/330 (78%)	243 (95%)	13 (5%)	21	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	261/330 (79%)	246 (94%)	15 (6%)	18	36
2	H	95/191 (50%)	91 (96%)	4 (4%)	26	49
2	I	93/191 (49%)	86 (92%)	7 (8%)	12	24
3	L	90/188 (48%)	82 (91%)	8 (9%)	9	18
3	M	87/188 (46%)	80 (92%)	7 (8%)	11	21
All	All	882/1418 (62%)	828 (94%)	54 (6%)	17	33

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	73	LEU
1	A	78	LEU
1	A	85	ARG
1	A	118	ASN
1	A	144	VAL
1	A	250	ILE
1	A	263	THR
1	A	289	THR
1	A	328	TYR
1	A	343	TYR
1	A	351	SER
1	A	355	CYS
1	B	45	ARG
1	B	75	GLU
1	B	85	ARG
1	B	88	VAL
1	B	98	GLU
1	B	110	ARG
1	B	114	VAL
1	B	120	ILE
1	B	157	LEU
1	B	176	ASN
1	B	261	MET
1	B	266	GLU
1	B	294	CYS
1	B	297	GLN
1	B	342	LEU
2	H	2	VAL
2	H	5	VAL

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Mol	Chain	Res	Type
2	H	31	SER
2	H	50	TYR
2	I	4	LEU
2	I	25	SER
2	I	50	TYR
2	I	78	LEU
2	I	109	MET
2	I	116	THR
2	I	120	VAL
3	L	2	ILE
3	L	11	LEU
3	L	22	THR
3	L	24	GLN
3	L	63	SER
3	L	81	GLU
3	L	104	LYS
3	L	107	ILE
3	M	2	ILE
3	M	10	SER
3	M	14	SER
3	M	17	ASP
3	M	30	SER
3	M	33	LEU
3	M	106	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	176	ASN
1	A	320	ASN
1	A	344	ASN
1	A	345	GLN
1	A	346	HIS
1	A	381	ASN
1	B	166	GLN
1	B	177	ASN
1	B	251	HIS
1	B	345	GLN
1	B	381	ASN
2	H	81	GLN
2	H	83	ASN

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Mol	Chain	Res	Type
2	I	3	GLN
2	I	39	GLN
3	L	24	GLN
3	L	79	GLN
3	M	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	C	1	4,1	14,14,15	0.29	0	17,19,21	0.58	0
4	NAG	C	2	4	14,14,15	0.29	0	17,19,21	0.46	0
4	NAG	D	1	4,1	14,14,15	0.31	0	17,19,21	0.78	0
4	NAG	D	2	4	14,14,15	0.32	0	17,19,21	1.04	2 (11%)
4	NAG	E	1	4,1	14,14,15	0.30	0	17,19,21	0.90	1 (5%)
4	NAG	E	2	4	14,14,15	0.27	0	17,19,21	0.51	0
4	NAG	X	1	4,1	14,14,15	0.38	0	17,19,21	0.70	1 (5%)
4	NAG	X	2	4	14,14,15	0.34	0	17,19,21	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	C1-O5-C5	2.97	116.16	112.19
4	D	2	NAG	C2-N2-C7	2.63	126.42	122.90
4	D	2	NAG	C1-O5-C5	2.15	115.07	112.19
4	X	1	NAG	C1-O5-C5	2.12	115.03	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

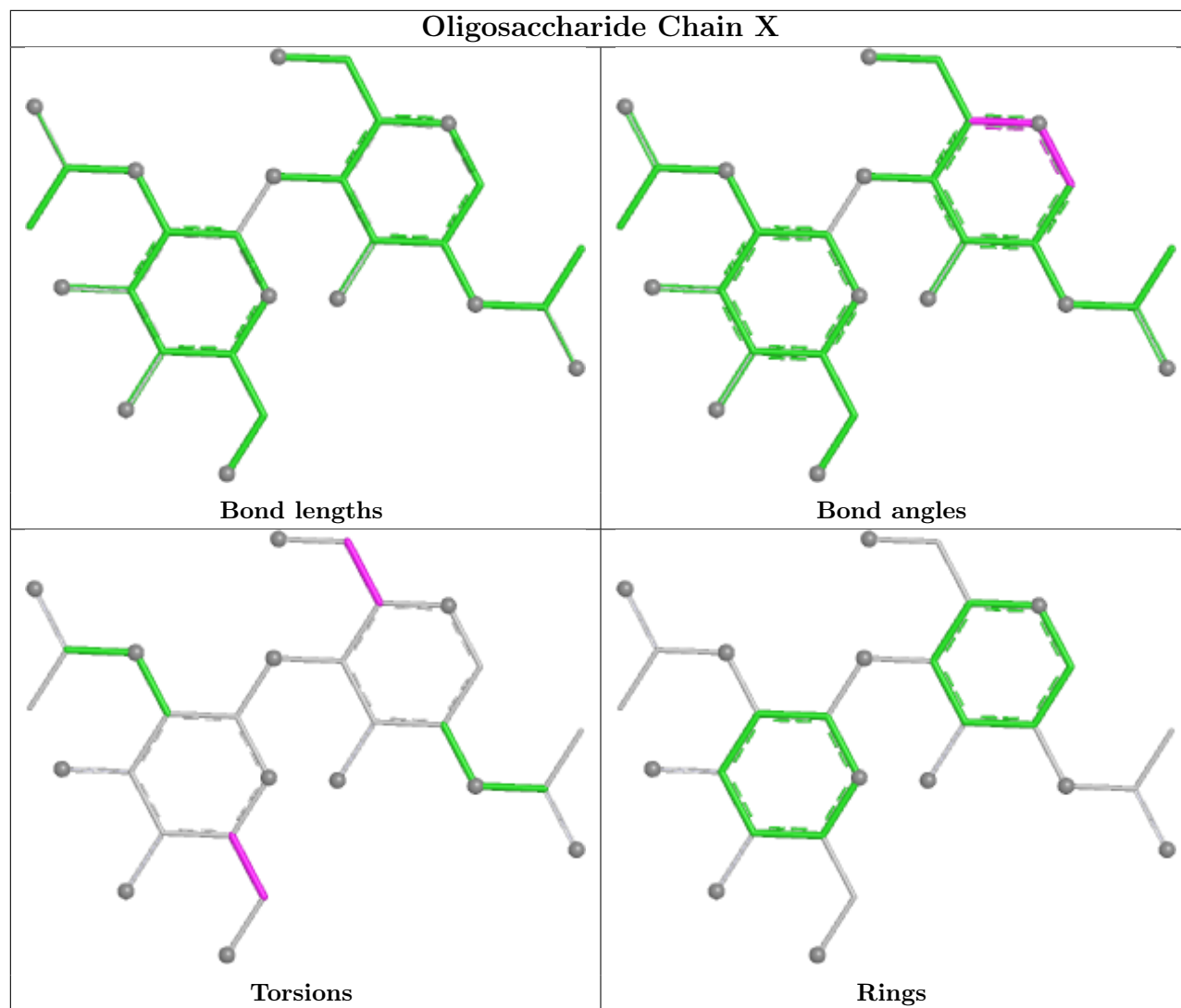
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C3-C2-N2-C7
4	X	2	NAG	O5-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C1-C2-N2-C7
4	X	1	NAG	C4-C5-C6-O6

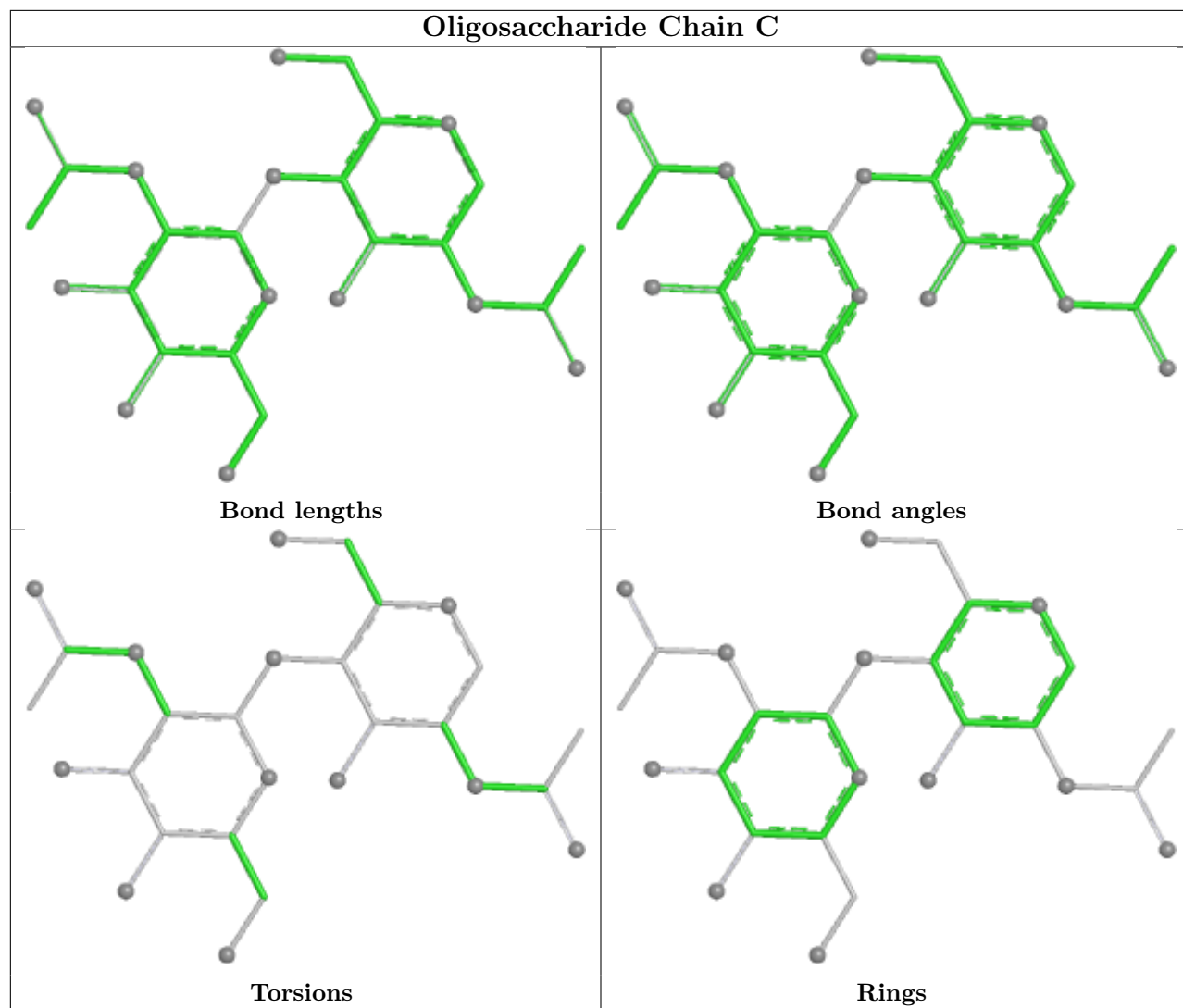
There are no ring outliers.

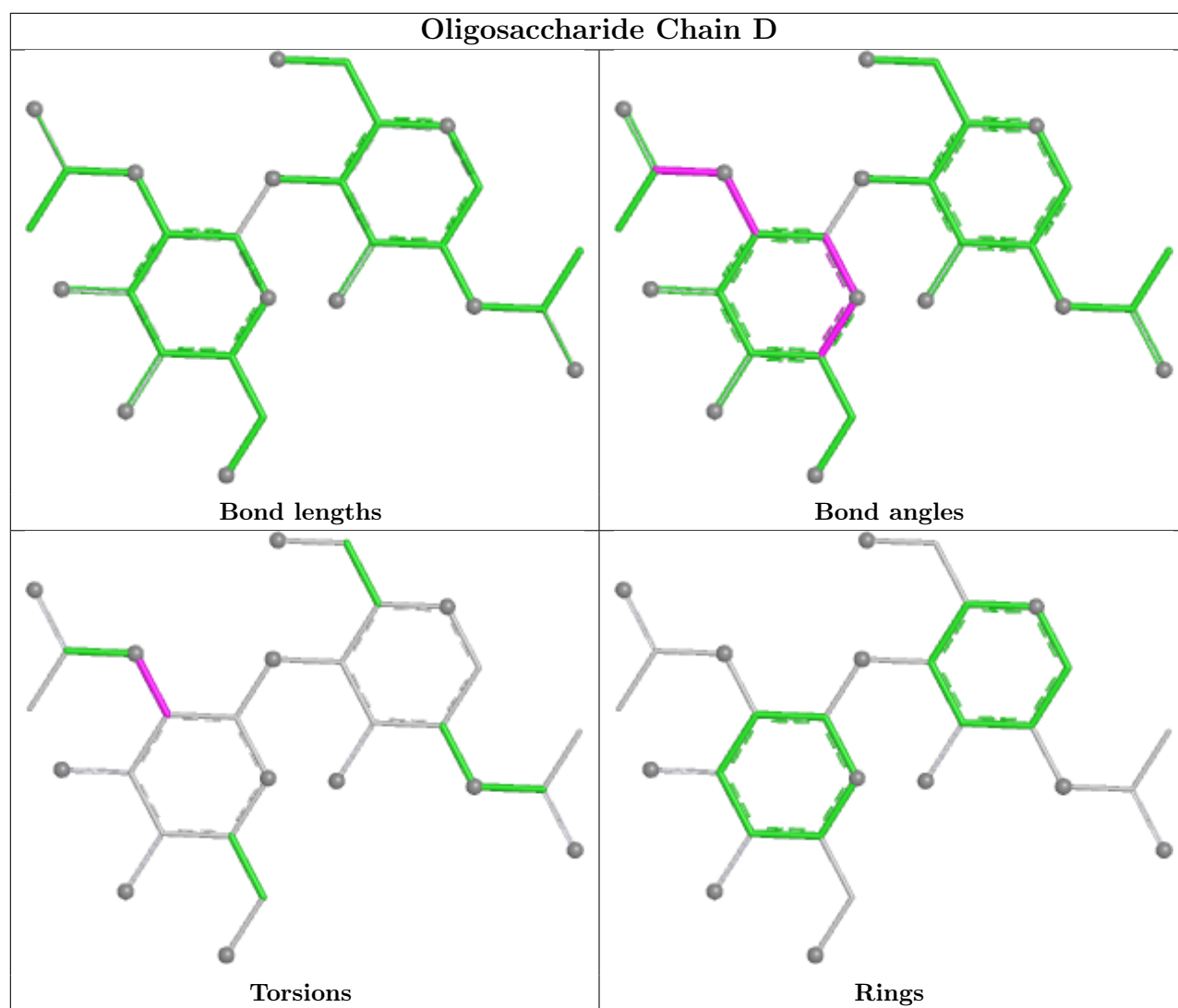
1 monomer is involved in 1 short contact:

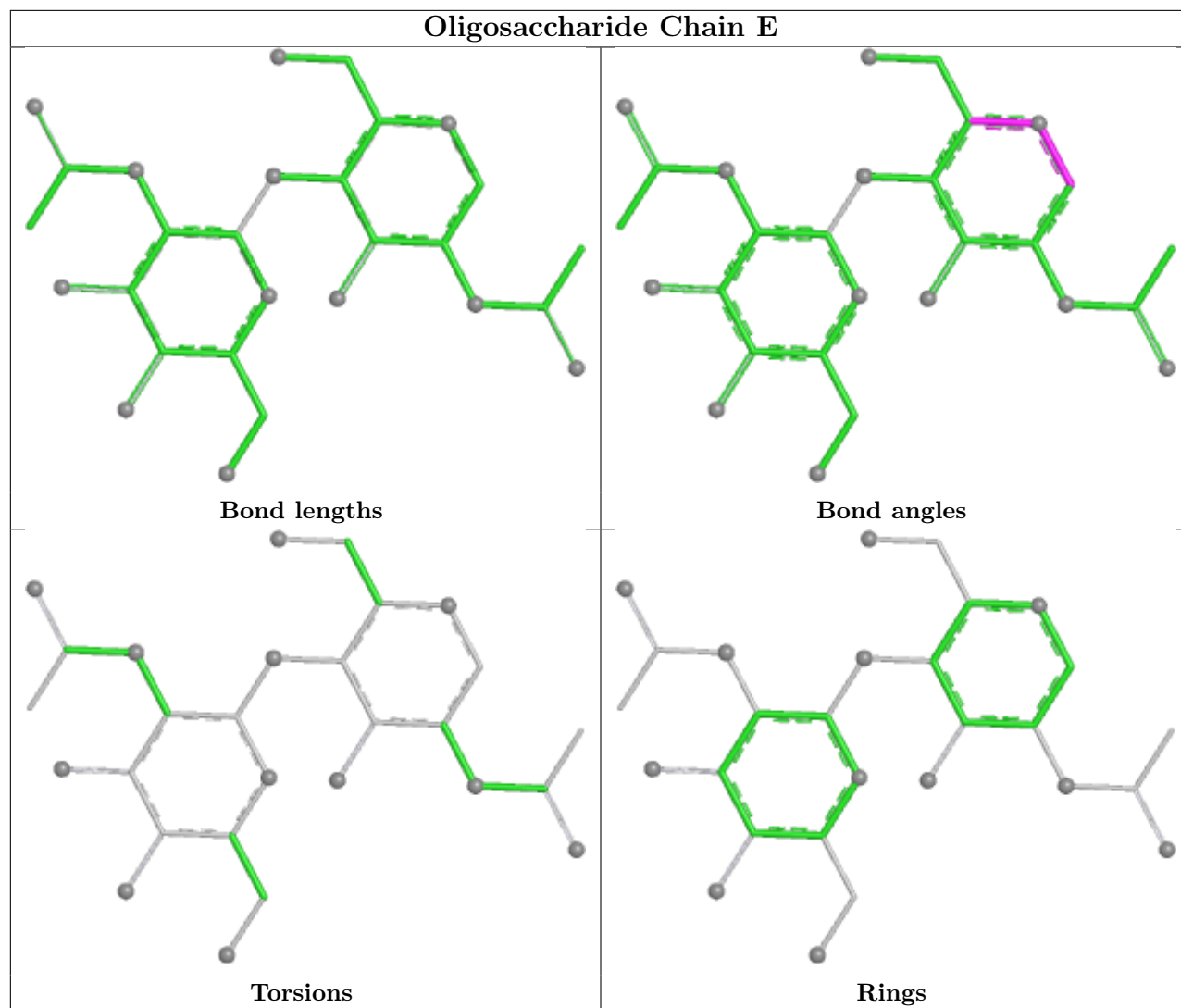
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	303/369 (82%)	1.56	79 (26%) 1 1	52, 77, 107, 114	0
1	B	317/369 (85%)	1.40	76 (23%) 2 1	44, 72, 105, 118	0
2	H	122/227 (53%)	1.20	17 (13%) 6 5	46, 77, 98, 106	0
2	I	121/227 (53%)	1.89	48 (39%) 1 0	62, 90, 106, 110	0
3	L	107/215 (49%)	0.82	9 (8%) 17 14	44, 65, 84, 87	0
3	M	107/215 (49%)	1.68	28 (26%) 1 1	65, 84, 104, 112	0
All	All	1077/1622 (66%)	1.45	257 (23%) 2 1	44, 77, 105, 118	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	ASN	10.0
1	A	95	PRO	8.1
1	A	343	TYR	7.2
1	B	280	LEU	6.7
2	I	11	VAL	6.1
3	M	92	SER	5.8
1	A	328	TYR	5.8
1	A	352	ALA	5.8
3	M	2	ILE	5.6
1	B	37	ASP	5.5
1	A	96	GLU	5.3
3	M	33	LEU	5.3
1	A	342	LEU	5.3
1	B	331	SER	5.2
1	A	347	ASN	5.0
2	I	118	VAL	5.0
1	A	134	PHE	5.0
1	B	287	SER	4.9
1	A	93	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	351	SER	4.8
1	B	60	ALA	4.8
1	B	50	ARG	4.6
1	A	300	ILE	4.5
1	B	283	ASN	4.5
1	B	310	TRP	4.5
1	A	99	PRO	4.5
1	A	345	GLN	4.4
2	I	94	TYR	4.4
2	I	47	TRP	4.3
1	B	246	ASP	4.3
3	M	3	GLN	4.3
1	B	248	ALA	4.2
1	B	368	TYR	4.1
1	B	99	PRO	4.1
2	I	119	THR	4.1
1	B	160	LEU	4.1
1	B	330	TRP	4.1
2	H	120	VAL	4.0
2	I	10	GLY	4.0
1	B	219	LEU	4.0
1	B	124	PHE	3.9
1	A	37	ASP	3.9
1	B	226	ASP	3.9
3	M	1	ASP	3.9
1	B	373	LYS	3.9
2	I	26	GLY	3.8
3	L	19	VAL	3.8
1	B	126	GLN	3.8
1	B	284	TYR	3.8
3	M	99	PHE	3.8
1	A	73	LEU	3.8
1	B	131	ILE	3.8
2	I	12	VAL	3.7
1	A	100	GLU	3.7
1	B	157	LEU	3.7
3	M	97	VAL	3.7
2	I	87	ALA	3.6
1	B	311	ILE	3.6
2	I	88	GLU	3.6
1	A	101	ALA	3.6
1	A	125	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	120	ILE	3.6
1	A	94	GLU	3.5
1	A	323	LEU	3.5
2	I	18	LEU	3.4
2	I	40	PRO	3.4
1	A	70	PRO	3.4
2	I	62	TRP	3.3
1	B	38	MET	3.3
2	H	122	SER	3.3
1	B	343	TYR	3.3
1	A	359	GLN	3.3
1	A	247	LEU	3.3
1	B	340	LEU	3.3
2	I	120	VAL	3.3
2	I	82	MET	3.3
3	M	107	ILE	3.3
1	B	317	TYR	3.3
1	B	127	SER	3.2
2	I	67	PHE	3.2
2	I	27	PHE	3.2
1	B	39	GLU	3.2
1	B	166	GLN	3.2
1	B	247	LEU	3.2
1	A	77	VAL	3.2
1	A	60	ALA	3.2
1	A	179	TRP	3.2
1	A	327	PRO	3.2
3	M	98	GLY	3.2
1	B	288	SER	3.1
3	L	107	ILE	3.1
2	H	121	SER	3.1
3	M	91	TYR	3.1
1	B	323	LEU	3.1
1	B	128	THR	3.1
2	I	45	LEU	3.1
2	H	77	THR	3.0
1	A	87	ARG	3.0
2	H	13	GLN	3.0
2	I	108	VAL	3.0
1	B	95	PRO	3.0
3	M	40	PRO	3.0
1	A	119	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	370	VAL	2.9
1	A	249	THR	2.9
2	I	86	ARG	2.9
2	H	116	THR	2.9
1	A	65	GLN	2.9
1	B	289	THR	2.9
2	I	29	PHE	2.9
2	I	121	SER	2.9
3	M	96	SER	2.9
3	M	88	CYS	2.8
2	I	36	TRP	2.8
2	I	46	GLU	2.8
1	A	123	LYS	2.8
1	B	120	ILE	2.8
1	B	370	VAL	2.8
2	H	22	CYS	2.8
1	B	64	SER	2.8
1	A	69	PRO	2.8
1	A	318	HIS	2.8
1	B	181	TYR	2.7
3	L	80	PRO	2.7
3	M	105	VAL	2.7
2	I	117	LEU	2.7
1	B	359	GLN	2.7
3	M	23	CYS	2.7
1	B	176	ASN	2.7
1	B	309	LYS	2.7
1	B	123	LYS	2.7
2	I	23	ALA	2.7
1	A	246	ASP	2.7
1	A	216	GLY	2.7
1	A	311	ILE	2.7
2	I	75	LYS	2.6
1	B	68	VAL	2.6
3	M	90	SER	2.6
1	A	181	TYR	2.6
2	H	24	ALA	2.6
1	A	147	PRO	2.6
1	A	321	PHE	2.6
3	M	51	ALA	2.6
1	B	129	HIS	2.6
1	A	291	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	I	44	GLY	2.6
1	A	376	VAL	2.6
1	A	348	PRO	2.6
2	I	102	TYR	2.6
1	B	329	ILE	2.5
1	B	213	GLU	2.5
1	A	178	SER	2.5
1	A	325	PRO	2.5
2	I	41	PRO	2.5
1	B	250	ILE	2.5
3	L	78	LEU	2.5
1	B	249	THR	2.5
1	B	390	SER	2.5
2	I	84	SER	2.5
3	L	21	ILE	2.5
1	B	125	LYS	2.5
1	A	353	ALA	2.5
1	B	293	CYS	2.5
1	A	67	GLU	2.5
1	B	98	GLU	2.5
1	B	369	TYR	2.5
1	A	217	PHE	2.5
1	B	308	TRP	2.5
1	A	175	SER	2.5
1	B	375	LYS	2.4
1	A	297	GLN	2.4
1	A	346	HIS	2.4
1	B	372	ARG	2.4
1	A	41	VAL	2.4
1	A	104	TYR	2.4
2	I	3	GLN	2.4
2	I	93	TYR	2.4
3	M	89	GLN	2.4
3	M	9	SER	2.4
1	B	222	HIS	2.4
1	A	74	PRO	2.4
1	B	63	PRO	2.4
1	A	121	TYR	2.4
2	H	61	ASN	2.4
2	I	107	TRP	2.4
2	I	112	TRP	2.4
2	I	122	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	253	MET	2.3
2	I	43	LYS	2.3
1	B	70	PRO	2.3
1	A	390	SER	2.3
2	H	1	GLN	2.3
3	M	10	SER	2.3
1	B	40	LEU	2.3
2	I	20	LEU	2.3
3	M	4	MET	2.3
3	M	93	ASP	2.3
1	A	174	TYR	2.3
2	I	2	VAL	2.3
1	B	93	ALA	2.3
1	B	303	ARG	2.3
2	I	49	GLY	2.3
1	A	72	PRO	2.3
1	A	267	ARG	2.3
1	A	116	THR	2.2
2	H	10	GLY	2.2
1	A	92	SER	2.2
1	A	253	MET	2.2
2	I	37	ILE	2.2
3	M	104	LYS	2.2
2	H	42	GLY	2.2
1	B	59	LEU	2.2
2	H	37	ILE	2.2
1	A	68	VAL	2.2
3	L	13	ALA	2.2
1	A	173	LYS	2.2
3	L	75	ILE	2.2
3	M	12	SER	2.2
1	A	98	GLU	2.2
2	I	19	ARG	2.2
1	A	219	LEU	2.2
1	B	73	LEU	2.2
2	H	79	TYR	2.2
3	M	78	LEU	2.2
1	B	100	GLU	2.2
3	L	1	ASP	2.2
1	B	69	PRO	2.2
1	A	135	PHE	2.2
1	B	161	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	208	LEU	2.1
3	M	41	GLY	2.1
3	M	87	TYR	2.1
2	I	5	VAL	2.1
2	H	27	PHE	2.1
1	B	65	GLN	2.1
1	A	350	ALA	2.1
2	I	63	ALA	2.1
2	I	61	ASN	2.1
1	A	180	ARG	2.1
1	A	326	CYS	2.1
1	A	97	PRO	2.1
1	B	164	VAL	2.1
2	H	11	VAL	2.1
1	A	207	TRP	2.1
1	B	90	GLY	2.1
2	I	90	THR	2.1
3	L	2	ILE	2.1
1	B	133	MET	2.1
1	B	88	VAL	2.0
2	I	38	ARG	2.0
1	B	252	GLY	2.0
1	A	209	SER	2.0
1	A	251	HIS	2.0
2	H	86	ARG	2.0
3	M	83	PHE	2.0
2	I	55	GLY	2.0
1	A	261	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

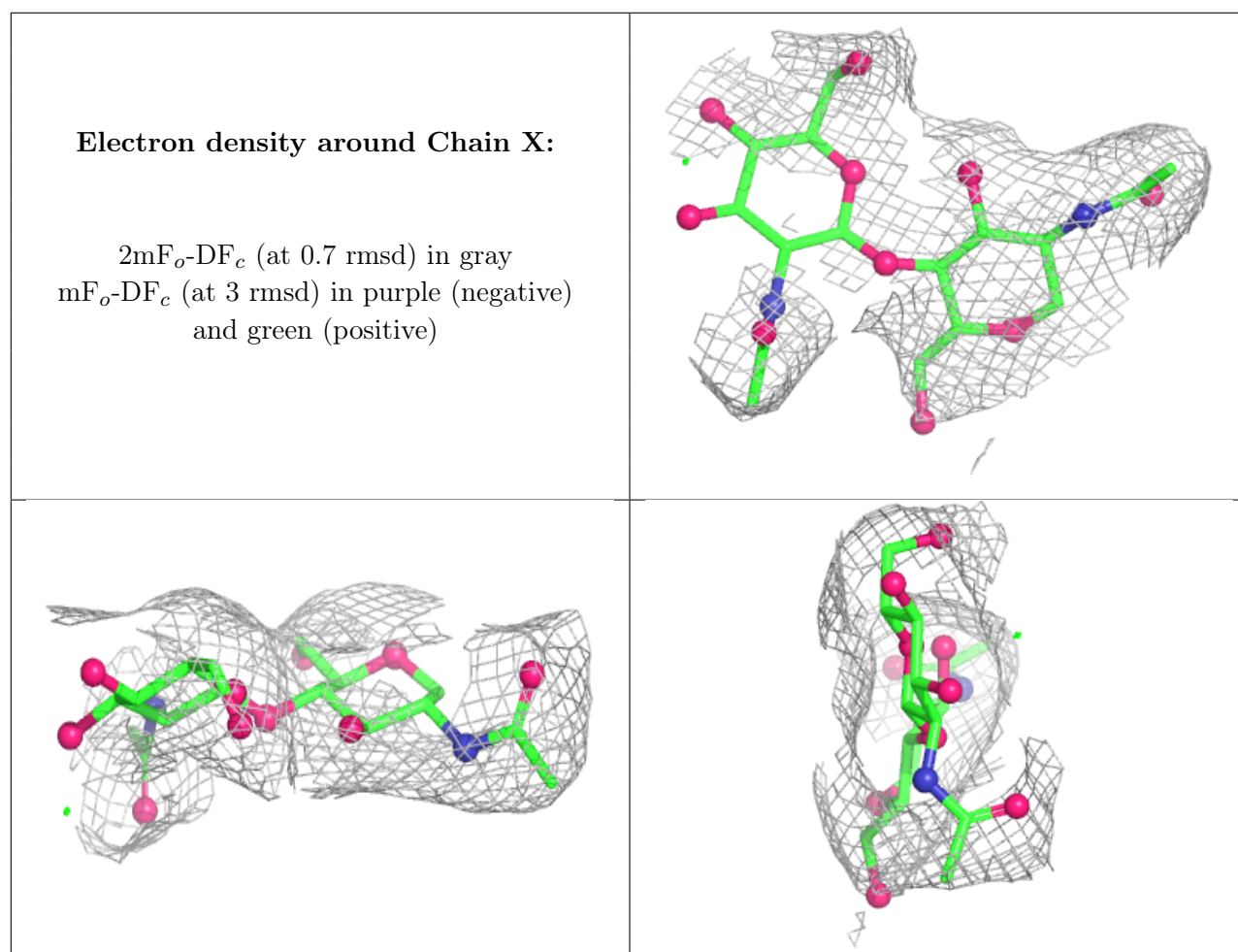
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

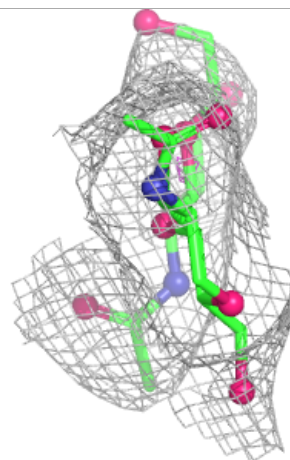
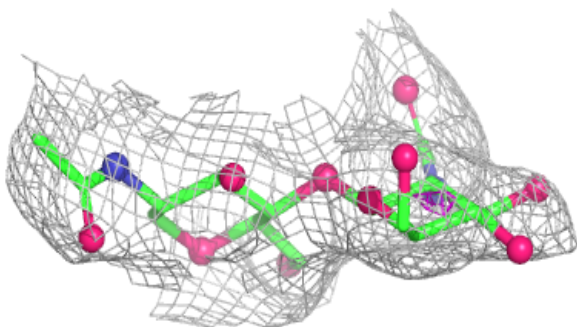
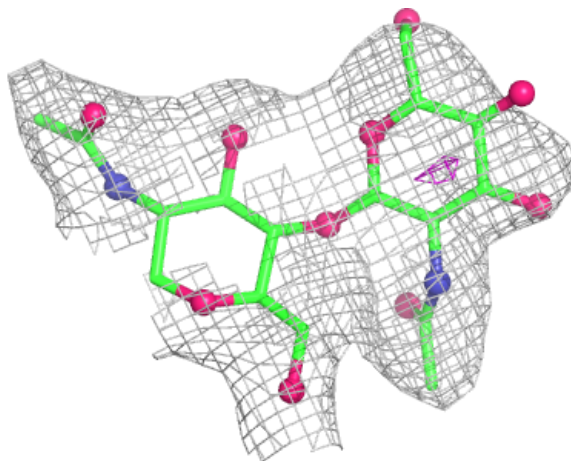
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	X	1	14/15	-	-	84,86,88,89	0
4	NAG	X	2	14/15	-	-	90,91,93,93	0
4	NAG	C	1	14/15	-	-	107,108,109,110	0
4	NAG	C	2	14/15	-	-	111,112,112,112	0
4	NAG	D	1	14/15	-	-	93,95,97,99	0
4	NAG	D	2	14/15	-	-	101,102,103,104	0
4	NAG	E	1	14/15	-	-	106,107,109,111	0
4	NAG	E	2	14/15	-	-	112,113,113,114	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



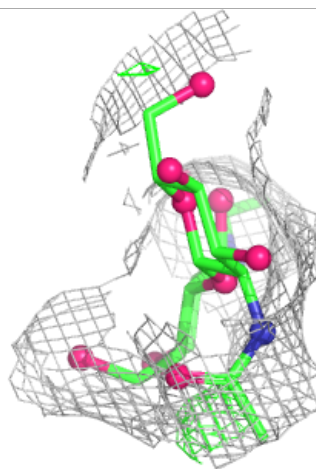
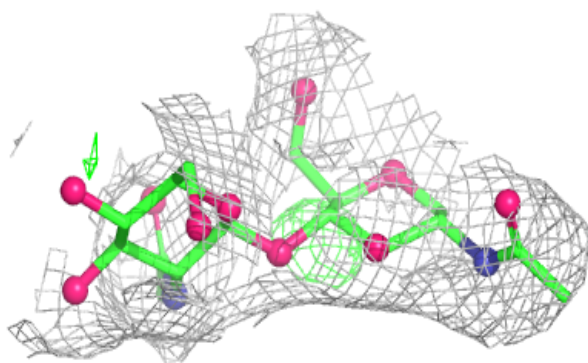
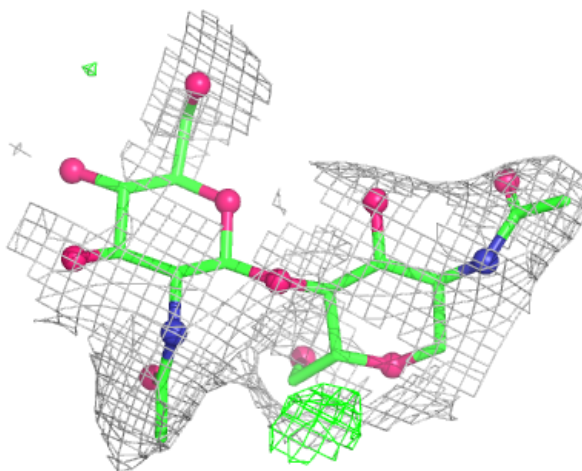
Electron density around Chain C:

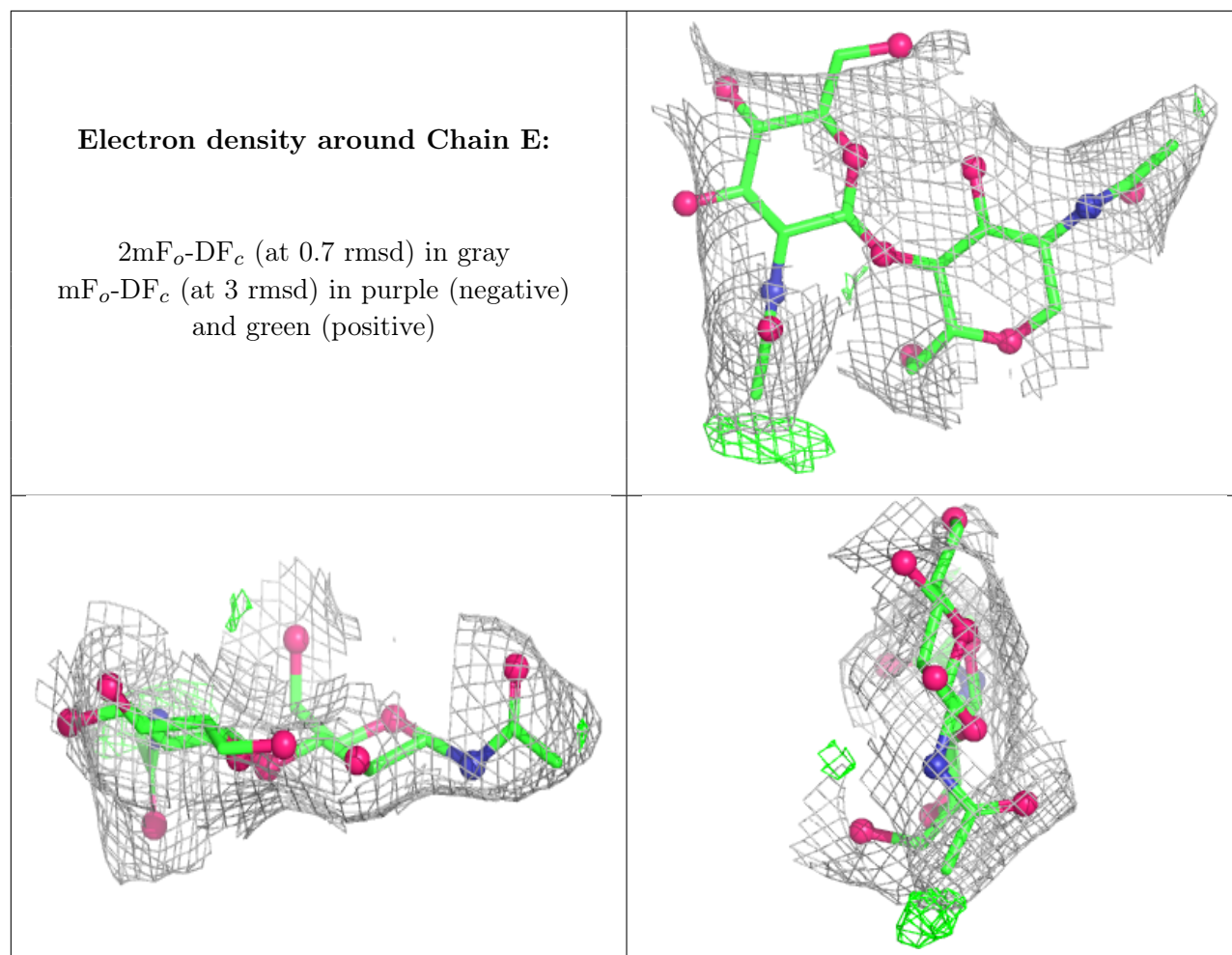
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.